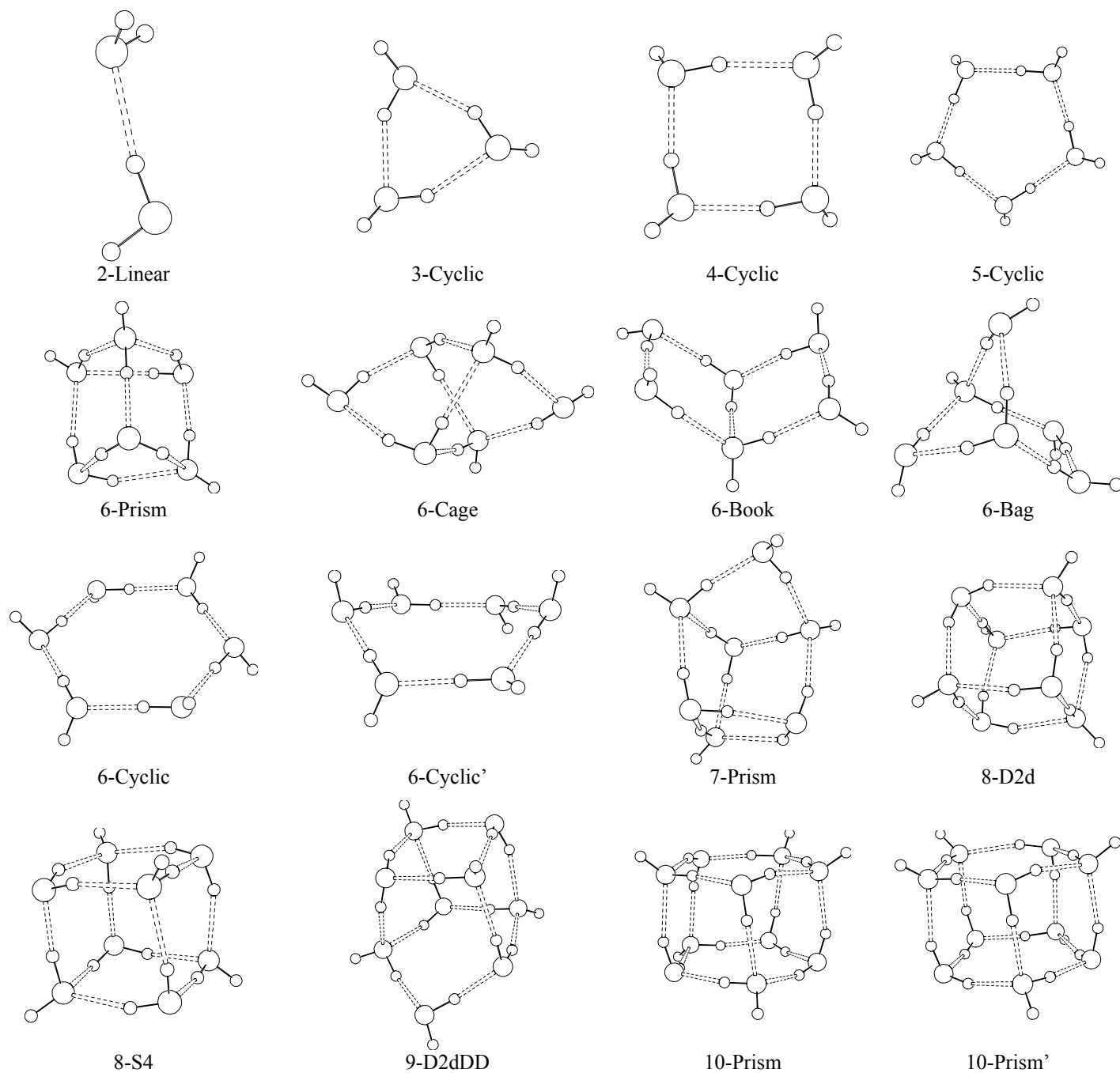


Table S1. Absolute energies (X3LYP/aug-cc-pVTZ(-f)), zero point energies, enthalpy, entropy, and dispersion contributions (as estimated by correlation portion of density functional).

# waters	Geometry	# dangling	# hbonds	E hartree	ZPE kcal/mol	H kcal/mol	S cal/(mol K)	E (no dispers.) hartree	frac disp	$\Delta E/n$ kcal/mol	$\Delta E/Hbond$ kcal/mol
1	Monomer	2	0	-76.435121	13.374	2.372	46.463	-76.028455			
2	Linear	3	1	-152.878205	28.892	4.254	69.623	-152.060983	0.49	-2.50	-5.00
3	Cyclic	3	3	-229.330099	45.677	5.257	79.399	-228.09732	0.52	-5.17	-5.17
4	Cyclic	4	4	-305.784676	61.973	6.585	91.446	-304.137045	0.47	-6.93	-6.93
5	Cyclic	5	5	-382.233878	77.407	8.485	108.808	-380.174039	0.45	-7.31	-7.31
6	Prism	3	9	-458.681951	94.277	9.715	115.415	-456.20379	0.54	-7.45	-4.97
6	Cage	4	8	-458.682091	94.16	9.696	115.496	-456.204527	0.53	-7.46	-5.60
6	Book	5	7	-458.682705	93.736	9.908	119.831	-456.207498	0.49	-7.53	-6.45
6	Bag	5	7	-458.681461	93.582	9.957	119.475	-456.206096	0.50	-7.40	-6.34
6	Cyclic	6	6	-458.682495	93.054	10.302	124.926	-456.210127	0.45	-7.51	-7.51
6	Cyclic'	6	6	-458.681005	92.704	10.511	127.516	-456.208941	0.46	-7.35	-7.35
7	Prism'	4	10	-535.13392	110.566	11.071	126.366	-532.241051	0.52	-7.90	-5.53
8	D2d	4	12	-611.594201	127.725	11.918	130.548	-608.281721	0.52	-8.88	-5.92
8	S4	4	12	-611.594672	127.786	11.856	130.317	-608.281531	0.53	-8.92	-5.95
9	D2dDD	5	13	-688.04415	143.292	13.71	145.548	-684.318835	0.51	-8.93	-6.18
10	Prism	5	15	-764.496491	159.558	15.149	155.501	-760.356014	0.51	-9.12	-6.08
10	Prism'	5	15	-764.497536	159.65	15.054	154.952	-760.356269	0.51	-9.18	-6.12
10	Butterfly	5	15	-764.485256	158.171	15.58	160.755	-760.349539	0.52	-8.41	-5.61
11	Pr443	5	17	-840.942162				-836.386975	0.53	-8.89	-5.75
12	Pr444	4	20	-917.400158				-912.424193	0.54	-9.34	-5.61
13	Pr454	5	21	-993.85164				-988.464362	0.52	-9.42	-5.83
14	Pr2444	5	23	-1070.304945				-1064.501895	0.51	-9.56	-5.82
15	Pr555	5	25	-1146.753647				-1140.537483	0.51	-9.49	-5.69
16	Pr4444	4	28	-1223.205892				-1216.571074	0.53	-9.57	-5.47
17	Pr454(4)	5	29	-1299.657127				-1292.60718	0.53	-9.60	-5.63
18	Pr44244	5	31	-1376.112089				-1368.645004	0.53	-9.76	-5.67
19	Globular	7	31	-1452.560728				-1444.680027	0.52	-9.69	-5.94

Table S2. Ball and stick drawings of water clusters studied.



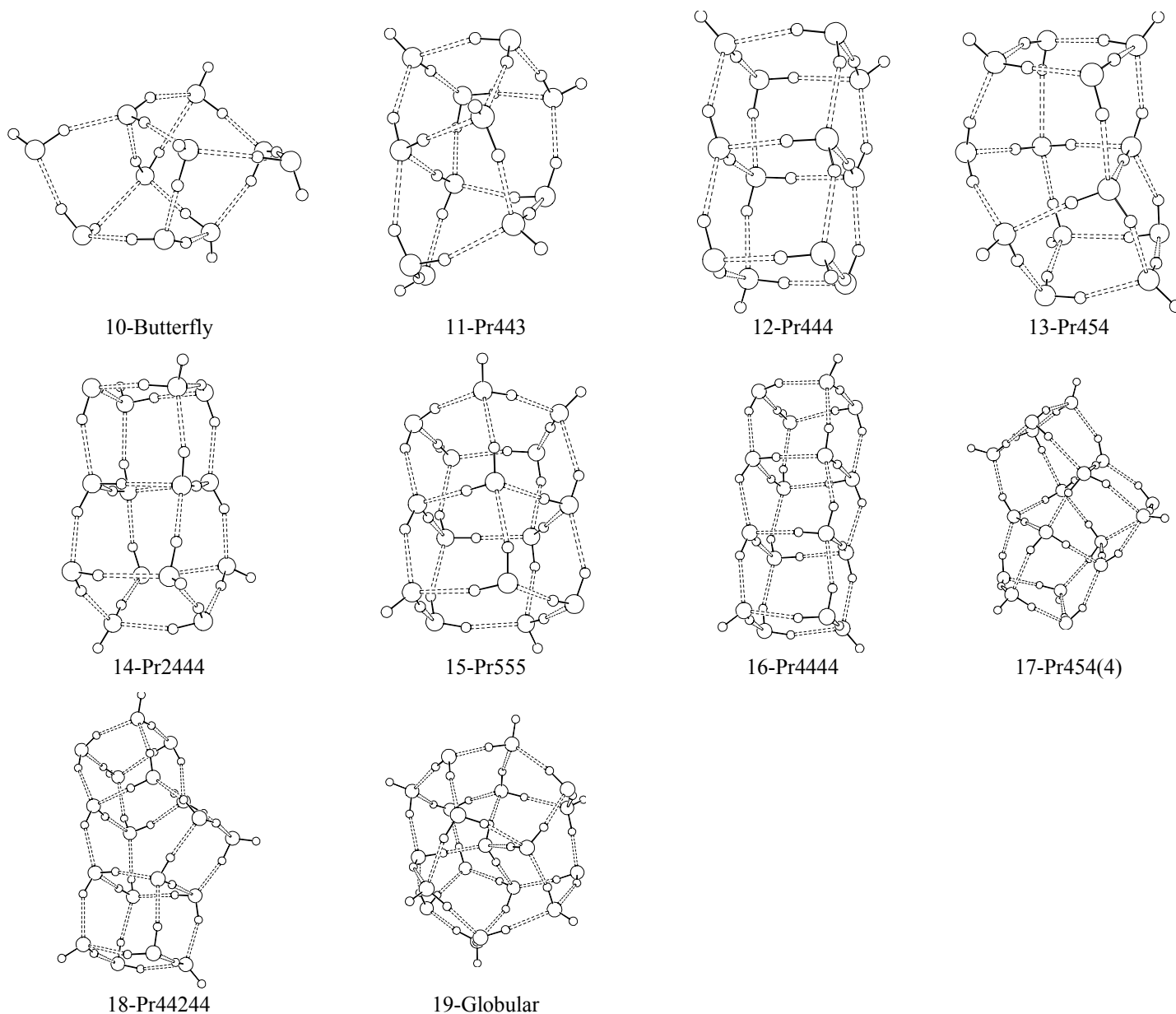


Table S3. Coordinates of water clusters studied.

1-Monomer	O -0.051900 -0.039920 0.000000 H -0.053040 0.921380 0.000000 H 0.876770 -0.287890 0.000000	2-Linear	O -0.200650 -1.268870 0.821330 H -0.160480 -1.088070 1.763710 H -0.064560 -0.412850 0.387630 O 0.181580 1.155100 -0.753860 H -0.584730 1.255510 -1.327550 H 0.925610 1.004230 -1.345560
3-Cyclic	O 1.213410 1.074900 -0.002530 H 0.529310 0.905700 0.670960 H 2.057630 1.029020 0.454080 O -1.103320 0.026080 1.179760 H -1.256770 -0.563830 1.922410 H -1.025070 -0.542450 0.390960 O -0.126970 -1.069840 -1.206350 H 0.518460 -0.356030 -1.046110	4-Cyclic	O -1.434840 1.247100 -0.347350 H -0.479590 1.451580 -0.228790 H -1.902780 1.804050 0.280930 O -1.271440 -1.456710 0.034090 H -1.459120 -0.500510 -0.103330 H -1.672340 -1.912980 -0.710890 O 1.446470 -1.256130 0.253070 H 0.486280 -1.456900 0.174870

	H -0.499550 -0.901180 -2.076120		H 1.736760 -1.673490 1.068800 O 1.260090 1.466000 0.060130 H 1.452600 0.505890 0.157850 H 1.838650 1.779990 -0.640280
5-Cyclic	O -1.112420 -1.551030 1.313010 H -0.717140 -2.039910 2.040060 H -1.013040 -0.598040 1.546560 O -0.058140 -2.010940 -1.154480 H -0.755270 -2.415320 -1.677490 H -0.443680 -1.873030 -0.257310 O 0.716130 2.202100 -0.094960 H 0.911630 1.523940 -0.783470 H 1.571000 2.543990 0.180990 O -0.773810 1.085550 1.889170 H -0.233450 1.516010 1.185120 H -1.568500 1.619580 1.972550 O 1.248430 0.264060 -1.926420 H 1.058110 0.440280 -2.851410 H 0.775720 -0.571160 -1.704990	6-Prism	O 1.941030 -0.055300 -1.575050 H 2.183030 -0.014050 -0.625690 H 1.503070 -0.918660 -1.624090 O -1.786890 -0.269700 -0.464430 H -1.429710 0.364370 -1.108600 H -1.701050 0.212550 0.369870 O 1.877990 -0.283530 1.214610 H 1.358600 -1.073150 0.997960 H 1.213370 0.393230 1.421740 O -0.269940 1.680250 1.195050 H -0.331290 2.492350 1.705770 H -0.136780 1.945090 0.262830 O -0.032290 1.697170 -1.556790 H 0.747550 1.079900 -1.657640 H 0.036860 2.349230 -2.259250 O 0.260500 -2.095540 -0.380390 H -0.552130 -1.540170 -0.409450 H -0.036310 -3.009590 -0.376820
6-Cage	O -2.033430 0.818920 1.913320 H -2.047440 1.319370 2.733030 H -1.564890 1.374170 1.253080 O -0.532240 -1.330550 1.004820 H -1.122330 -0.720120 1.490340 H 0.348320 -0.938850 1.122320 O 1.804130 0.325810 0.589680 H 2.038080 -0.123670 -0.254290 H 2.628430 0.459360 1.065600 O -0.751130 -0.681910 -1.554390 H -1.461710 -1.135540 -2.016670 H -0.775360 -1.006700 -0.610310 O -0.526270 1.905300 -0.133230 H -0.772010 1.274330 -0.827110 H 0.357630 1.604970 0.135180 O 1.967280 -1.043090 -1.762540 H 2.350360 -0.688790 -2.569760 H 0.994900 -1.007210 -1.886870	6-Book	O -1.482840 -0.714630 -0.344050 H -2.370790 -0.864540 -0.008350 H -1.510960 0.162460 -0.781140 O 3.041960 -0.537180 0.238510 H 3.014590 -1.248410 -0.407440 H 2.150240 -0.524070 0.672850 O 0.644070 -0.158990 1.384130 H 0.588020 0.804990 1.291070 H -0.116670 -0.483940 0.862200 O 3.129580 2.028140 -0.503130 H 3.926610 2.415940 -0.131300 H 3.180860 1.060260 -0.293480 O -1.345090 1.855910 -1.339280 H -1.111230 2.056290 -2.249670 H -0.618630 2.213290 -0.789520 O 0.680840 2.588810 0.401100 H 0.655290 3.403400 0.911030 H 1.611890 2.487610 0.073460
6-Bag	O 2.472560 -2.539170 2.545030 H 3.009780 -2.544700 1.731320 H 1.571340 -2.344850 2.227830 O 3.736490 -2.019990 0.048730 H 4.667910 -1.792110 -0.014540 H 3.247870 -1.181340 -0.038780 O 2.432740 1.580540 2.407710 H 3.104140 2.265370 2.471170 H 2.708800 0.880360 3.055760 O 3.244380 -0.425370 3.950270 H 3.000820 -0.563020 4.869450 H 2.971470 -1.252820 3.465520 O 2.013290 0.220600 0.157030 H 2.206100 0.794370 0.945250 H 1.805540 0.815750 -0.569070 O 0.107180 -1.546640 1.308230 H -0.572680 -1.063650 1.786160 H 0.623060 -0.872710 0.829310	6-Cyclic	O 0.781380 2.576250 -0.025840 H -0.188640 2.410960 -0.105090 H 0.881180 3.188180 0.708380 O 1.421650 -2.039900 0.385840 H 1.817540 -2.349430 1.204970 H 1.769330 -1.125880 0.250650 O 2.430350 0.439490 0.041040 H 1.810160 1.207280 0.026100 H 2.991260 0.544170 -0.732140 O -1.240420 -2.435390 0.185030 H -1.339240 -3.052770 -0.544700 H -0.270470 -2.270070 0.264720 O -1.880600 2.180800 -0.226470 H -2.277000 2.495840 -1.043260 H -2.228720 1.266120 -0.096800 O -2.890420 -0.300140 0.103550 H -3.459560 -0.406630 0.870450 H -2.269900 -1.067550 0.123840
6-Cyclic'	O -2.144330 -0.798890 0.919070 H -2.101650 -0.538870 -0.031610 H -3.062970 -0.700650 1.180870 O 2.287650 -0.451280 1.334880 H 2.567330 -1.358950 1.481600 H 1.418810 -0.365250 1.794880	7-Prism'	O 0.458310 2.490940 0.826510 H 0.458060 3.257330 1.406250 H -0.468100 2.136880 0.819630 O -0.969510 -1.249760 1.502060 H -1.312570 -1.699400 2.279590 H -0.825080 -1.946420 0.818960

	O -0.097850 -0.234760 2.594970 H -0.863030 -0.412120 1.999300 H -0.272040 0.616910 3.004120 O 2.351950 0.426060 -1.226580 H 3.203780 0.858200 -1.325060 H 2.315960 0.101130 -0.295810 O -2.063950 -0.076040 -1.689410 H -2.151260 -0.784350 -2.333010 H -1.268660 0.437420 -1.968360 O 0.121050 1.319750 -2.465430 H 0.066820 2.269940 -2.333930 H 0.945660 1.028730 -2.010250		O 1.327570 -0.891640 -1.427950 H 2.180740 -1.034720 -1.848710 H 1.522860 -0.554760 -0.505430 O 1.590320 -0.045620 1.049270 H 1.361660 0.904580 1.072950 H 0.817890 -0.479970 1.450200 O -0.251800 -2.951010 -0.480920 H 0.343870 -2.329110 -0.951210 H -0.874770 -3.268960 -1.140510 O -1.877290 1.262350 0.417810 H -1.601070 1.192200 -0.515530 H -1.752970 0.372110 0.786360 O -0.316030 1.455220 -1.926320 H 0.254310 0.668510 -1.941430 H 0.176480 2.097770 -1.399190
8-D2d	O 1.363030 -1.364550 1.453860 O -1.358000 -1.367950 -1.456430 O 1.363350 1.362710 -1.453460 O -1.359210 1.367660 1.457010 H 1.475540 -1.474240 0.469780 H -1.470630 -1.475100 -0.472110 H 1.474420 1.473660 -0.469320 H -1.471370 1.474730 0.472680 H 1.974430 -1.978830 1.870030 H -1.971120 -1.981630 -1.871030 H 1.972660 1.979230 -1.869390 H -1.970890 1.982910 1.871280 O 1.466980 -1.463970 -1.197610 O -1.461450 -1.461060 1.195660 O 1.465440 1.463430 1.198010 O -1.461460 1.460330 -1.195000 H 0.538810 -1.615190 -1.451860 H -0.532690 -1.610780 1.448850 H 0.537050 1.613850 1.452120 H 1.615620 -0.535360 -1.451610 H -1.607420 0.530940 -1.447590 H 1.613600 0.534480 1.450920 H -1.609920 -0.532170 1.448550 H -0.533010 1.612540 -1.447630	8-S4	O -1.314570 -1.318060 0.132320 H -0.561920 -1.418770 -0.514720 H -1.729730 -2.182510 0.201560 O -0.237630 0.947500 -2.870780 H -0.152010 1.206100 -3.792850 H 0.287880 1.610830 -2.342890 O 1.093210 2.584080 -1.267600 H 1.702650 1.962540 -0.828230 O 0.459200 2.818310 -0.566840 O 0.730590 -1.345960 -1.549250 H 0.455110 -0.668450 -2.194220 H 1.458340 -0.919180 -1.063350 O 0.363220 0.237540 1.843640 H -0.243850 -0.433810 1.485250 H -0.106070 1.078370 1.688920 O -0.901960 2.514020 0.770040 H -1.514870 2.027840 0.150820 H -1.435260 3.181320 1.211320 O 2.308300 0.410380 0.052740 H 1.642790 0.338290 0.792280 H 3.176120 0.349630 0.462100 O -2.333320 1.081130 -0.934960 H -2.192690 0.182120 -0.583820 H -1.821140 1.087570 -1.762720
9-D2dDD	O 0.228290 -3.096920 1.029720 H 0.441170 -3.976180 0.706770 H 0.974100 -2.504710 0.741620 O -1.029530 0.673490 1.945790 H -1.429540 1.282670 1.299950 H -1.308860 -0.196690 1.609920 O 2.115640 -1.389520 0.258000 H 2.086180 -0.609360 0.840800 H 1.934160 -1.010630 -0.621070 O -1.859640 -1.611660 0.412640 H -1.150220 -2.275680 0.619860 H -2.698000 -2.037780 0.612100 O -1.792080 2.061540 -0.409580 H -0.848920 2.353410 -0.544160 H -2.344340 2.836200 -0.547760 O -1.315130 -0.253760 -1.994960 H -1.539610 -0.878680 -1.280870 H -1.641260 0.592400 -1.640320 O 1.574310 1.064380 1.587590 H 1.987890 1.367380 2.401020 H 0.617960 0.892190 1.806070 O 1.310710 0.089760 -2.036610 H 0.331660 -0.095800 -2.080110 H 1.649170 -0.037740 -2.927620 O 0.797040 2.554050 -0.705140 H 1.187560 2.260630 0.137980 H 1.087870 1.860580 -1.324680	10-Prism	O -0.001380 0.752460 2.303590 H 0.142980 -0.130970 1.863010 H 0.382270 0.683780 3.182660 O -2.775270 0.522180 1.540950 H -1.938380 0.583280 2.032740 H -2.774000 1.350740 1.024760 O 0.190640 -1.554280 1.028860 H -0.722020 -1.772060 0.764630 H 0.633330 -1.423480 0.170810 O -1.751050 -0.524370 -2.589510 H -2.158410 -0.912860 -1.795090 H -0.821530 -0.784510 -2.495860 O 1.239050 1.656320 -1.894410 H 2.023240 2.094740 -2.237390 H 1.064160 2.059580 -0.993440 O -2.448170 -1.577960 -0.042540 H -2.662010 -0.793970 0.534370 H -3.153850 -2.216400 0.096130 O 0.979580 -1.032200 -1.633660 H 1.191650 -0.076860 -1.752120 H 1.664190 -1.523620 -2.096490 O 0.616450 2.724550 0.418270 H 0.580280 2.063400 1.136320 H -0.313620 3.007700 0.350380 O -1.622170 2.218160 -2.367720 H -1.795760 1.258310 -2.503010 H -0.655880 2.265100 -2.427280 O -2.217120 2.873020 0.109490

				H -2.074350 2.643160 -0.853560	
				H -2.784720 3.649170 0.121530	
10-Prism'	O -1.920930 0.293030 2.043670		10-Butterfly	O -3.387150 0.864020 2.379180	
	H -2.061260 -0.657650 1.767420			H -3.572190 1.652270 2.896140	
	H -2.632830 0.496650 2.657360			H -2.438240 0.671510 2.499340	
	O 1.506210 1.459970 0.423390			O -1.937110 -1.916500 -0.828020	
	H 2.098360 2.166870 0.695500			H -2.561770 -1.186780 -0.629380	
	H 1.301740 0.932670 1.255130			H -1.306740 -1.503860 -1.443160	
	O 0.831160 0.117640 2.545040			O -0.607290 1.589970 -0.229370	
	H 0.928270 -0.850770 2.472830			H -0.845980 1.003780 0.517220	
	H -0.136560 0.248220 2.563230			H 0.238710 1.956810 0.063990	
	O -1.279920 1.620610 -0.396220			O -0.755090 0.051280 2.138150	
	H -1.671560 1.247860 0.413170			H -0.709190 -0.910300 1.973880	
	H -0.360170 1.799220 -0.144070			H 0.179130 0.336530 2.161390	
	O 1.935330 -0.337250 -1.543400			O -0.074980 -0.192290 -2.183440	
	H 2.706660 -0.111800 -2.071370			H -0.252210 0.163660 -3.059300	
	H 1.873660 0.353260 -0.840260			H -0.299190 0.524470 -1.539540	
	O -1.364760 -2.641020 -1.335140			O 1.749200 0.924740 1.386440	
	H -1.827970 -3.160940 -1.998610			H 2.028950 0.338770 0.631320	
	H -1.227280 -1.733470 -1.743830			H 2.557600 1.157780 1.850910	
	O -0.841420 -0.291820 -2.333570			O -0.507310 -2.626800 1.234340	
	H 0.128580 -0.256410 -2.301090			H -1.110290 -2.405430 0.463490	
	H -1.116470 0.412550 -1.703490			H -0.932920 -3.346110 1.711200	
	O 1.300930 -2.902310 -0.471110			O -3.399270 0.431260 -0.375580	
	H 1.674260 -2.079410 -0.833780			H -3.553630 0.625600 0.569830	
	H 0.421550 -2.970190 -0.889270			H -2.834210 1.154300 -0.670200	
	O 0.619860 -2.646740 2.050680			O 1.773490 -3.243670 -0.331290	
	H 0.938120 -2.763390 1.109730			H 0.990730 -3.145140 0.244910	
	H 0.991150 -3.381660 2.547690			H 1.469670 -3.729240 -1.103800	
	O -2.102950 -2.239070 1.359210			O 2.381560 -0.548900 -0.742240	
	H -1.247980 -2.555560 1.701970			H 1.697270 -0.376010 -1.409440	
	H -2.038210 -2.397130 0.398420			H 2.305060 -1.512800 -0.594490	
11-Pr443	O -0.817360 0.686570 -1.815400		12-Pr444	O 1.794470 0.923410 2.768350	
	H -0.685500 0.309700 -2.709040			H 2.338250 1.359750 3.430940	
	H -1.653840 0.293910 -1.498220			H 0.879480 1.303000 2.865760	
	O -2.034010 1.253400 2.685060			O -1.794470 -0.923410 2.768350	
	H -2.650730 1.679990 2.063510			H -2.338250 -1.359750 3.430940	
	H -2.207800 0.304570 2.560830			H -0.879480 -1.303000 2.865760	
	O -0.542520 -0.966550 -3.988220			O 0.923410 -1.794470 -2.768350	
	H -1.096780 -1.633730 -3.529550			H 1.359750 -2.338250 -3.430940	
	H -0.826990 -0.958350 -4.905740			H 1.303000 -0.879480 -2.865760	
	O -3.289200 -0.307920 -0.770470			O -1.752130 -0.741530 -2.896280	
	H -3.187310 -0.729450 0.100010			H -2.036450 -0.920500 -1.984040	
	H -3.611200 0.583830 -0.545390			H -0.921210 -1.242140 -2.984230	
	O -2.146480 -2.512730 -2.343220			O -0.885520 1.737840 0.052730	
	H -2.779010 -1.848310 -2.030690			H -1.032320 2.090180 -0.841890	
	H -1.669100 -2.765060 -1.535210			H -1.284090 0.839590 0.017130	
	O -0.891550 -2.762070 0.317020			O 0.885520 -1.737840 0.052730	
	H -0.409030 -3.553960 0.573010			H 1.284090 -0.839590 0.017130	
	H -0.209890 -2.026030 0.250230			H 1.032320 -2.090180 -0.841890	
	O 0.737400 -0.745510 0.042640			O 1.737840 0.885520 -0.052730	
	H 0.738540 -0.049120 0.723680			H 2.090180 1.032320 0.841890	
	H 0.350950 -0.278970 -0.726260			H 0.839590 1.284090 -0.017130	
	O -2.683110 -1.379830 1.842310			O -1.737840 -0.885520 -0.052730	
	H -2.027390 -1.992590 1.435550			H -2.090180 -1.032320 0.841890	
	H -3.306630 -1.927740 2.328440			H -0.839590 -1.284090 -0.017130	
	O 0.351710 1.638640 1.565050			O 1.752130 0.741530 -2.896280	
	H 0.982740 2.023760 2.180130			H 2.036450 0.920500 -1.984040	
	H -0.493220 1.506730 2.071010			H 0.921210 1.242140 -2.984230	
	O -1.168360 3.074140 -0.468740			O 0.741530 -1.752130 2.896280	
	H -0.539270 2.813000 0.226170			H 0.920500 -2.036450 1.984040	
	H -0.996290 2.410190 -1.164870			H 1.242140 -0.921210 2.984230	
	O -3.516530 2.225530 0.414420			O -0.923410 1.794470 -2.768350	
	H -4.187060 2.914380 0.390970			H -1.359750 2.338250 -3.430940	
	H -2.677090 2.633490 0.057820			H -1.303000 0.879480 -2.865760	
				O -0.741530 1.752130 2.896280	
				H -0.920500 2.036450 1.984040	

H -1.242140 0.921210 2.984230

13-Pr454 O 3.258030 4.399600 -1.977870
H 3.331370 3.544140 -2.432640
H 2.298740 4.529430 -1.872370
O 0.091140 -1.068930 -2.221390
H 0.333660 -1.458020 -1.362600
H 0.013490 -0.118240 -2.018080
O 5.011910 0.323760 -0.933070
H 4.597710 -0.581780 -1.002240
H 5.946900 0.211470 -1.127630
O 1.144940 3.946940 1.374580
H 2.106990 4.092990 1.315390
H 1.050040 3.008890 1.604110
O 0.515070 4.328700 -1.195010
H -0.166960 4.994960 -1.319040
H 0.667150 4.253980 -0.215370
O 1.370100 0.871960 1.219150
H 1.155820 1.168600 0.312270
H 2.333960 1.043970 1.340950
O 3.178190 1.589440 -2.673490
H 2.973110 0.840230 -3.261590
H 3.878500 1.240370 -2.087300
O 3.716680 -1.952160 -1.227330
H 2.964900 -1.974850 -0.607220
H 3.309450 -1.799900 -2.099120
O 3.879700 4.147100 0.634770
H 4.517840 4.822810 0.881660
H 3.736960 4.243930 -0.343600
O 0.686170 1.537420 -1.423540
H 0.358430 2.453380 -1.454800
H 1.566060 1.583280 -1.854240
O 1.308680 -1.710510 0.316830
H 1.020680 -2.340960 0.983910
H 1.305630 -0.824340 0.759790
O 4.053360 1.433880 1.495890
H 4.118610 2.380240 1.283490
H 4.505010 0.995940 0.754180
O 2.378340 -0.984340 -3.565650
H 2.307930 -1.422080 -4.419040
H 1.478460 -1.056610 -3.140720

14-Pr2444 O -4.474220 1.674100 -2.952740
H -5.233050 2.146470 -3.308410
H -4.720630 0.711160 -2.958700
O 2.032530 -1.970220 -2.046320
H 1.871450 -2.021600 -3.028850
H 2.987020 -1.974390 -1.928540
O 0.022770 -0.141910 -1.411790
H -0.579800 -0.863190 -1.117860
H 0.893950 -0.575340 -1.480990
O -1.852300 2.188720 -3.994000
H -1.486930 2.447710 -3.133150
H -2.794920 2.047190 -3.796640
O -3.990840 -1.103370 -0.002070
H -3.838670 -0.119720 -0.004020
H -4.514800 -1.291350 0.782060
O 0.240920 -4.247980 -1.633950
H -0.455360 -3.754760 -1.165000
H 0.983610 -3.620380 -1.651920
O -0.686000 -4.177310 -4.173080
H -0.353940 -4.311200 -3.247200
H -0.716610 -5.049260 -4.577810
O -1.649190 -2.270410 -0.946510
H -2.050650 -2.308060 -1.843230
H -2.398360 -2.003870 -0.381760
O -0.741270 -0.332370 -4.122220
H -1.119560 0.555240 -4.310760
H -0.435340 -0.233560 -3.199470
O -1.072470 2.334770 -1.150610
H -0.519460 2.982180 -0.703800
H -0.559210 1.496640 -1.164830
O -5.045790 -0.932410 -2.728380
H -4.365500 -1.466900 -3.175900
H -4.879780 -1.099730 -1.784820
O -3.664820 1.536000 -0.224410
H -2.748070 1.837280 -0.352720
H -4.078620 1.728750 -1.085810
O 1.350050 -2.134770 -4.621050
H 0.735110 -1.383160 -4.709710
H 0.760170 -2.907620 -4.663170
O -2.650420 -2.230130 -3.528380
H -2.258810 -3.038910 -3.901760
H -2.054690 -1.516480 -3.851010

15-Pr555 O -1.459300 -1.190050 -5.331450
H -1.883220 -1.380660 -6.173730
H -1.497720 -0.214470 -5.215990
O -2.196240 -1.603440 -2.546290
H -2.318950 -1.592810 -3.507230
H -1.304100 -2.002700 -2.441390
O -1.522470 1.493800 -4.687690
H -0.607320 1.801230 -4.431030
H -1.859420 2.154160 -5.300680
O -2.300920 0.658370 1.104810
H -2.538040 -0.277960 0.926250
H -2.419070 1.085060 0.242630
O 2.075840 -0.823210 -1.337090
H 2.621640 -0.635310 -2.117690
H 1.550480 0.002120 -1.234550
O -2.042280 1.064810 -1.805440
H -2.120210 0.107920 -2.016600
H -2.128280 1.488370 -2.672780
O 0.294040 0.709360 1.621090
H 0.448080 1.170910 2.451030
H -0.697180 0.692330 1.497210
O 1.260280 -2.047200 -4.888130
H 1.055650 -2.549230 -4.079780
H 0.381340 -1.755370 -5.187940

16-Pr4444 O 1.461480 -1.327600 -1.353220
H 1.752410 -1.515580 -2.262910
H 0.494650 -1.478150 -1.385430
O 1.461480 1.327600 1.353220
H 0.494650 1.478150 1.385430
H 1.752410 1.515580 2.262910
O 1.089520 -1.564070 4.334860
H 1.349150 -1.797040 3.427240
H 1.399750 -0.645990 4.429810
O 1.358940 -1.480240 1.495220
H 1.496100 -0.511150 1.433610
H 1.671650 -1.803630 0.636070
O -1.358940 1.480240 1.495220
H -1.496100 0.511150 1.433610
H -1.671650 1.803630 0.636070
O -1.089520 -1.564070 -4.334860
H -1.349150 -1.797040 -3.427240
H -1.399750 -0.645990 -4.429810
O -1.564130 1.283130 -4.175150
H -2.024300 1.818770 -4.828060
H -0.594190 1.470250 -4.292410
O -1.564130 -1.283130 4.175150
H -0.594190 -1.470250 4.292410
H -2.024300 -1.818770 4.828060

O 0.315810 -2.726630 -2.292910
H 0.927370 -2.054350 -1.916810
H 0.129730 -3.325080 -1.547660
O 0.609750 1.500370 -1.095110
H 0.640860 1.542930 -0.123330
H -0.333520 1.323330 -1.302450
O -2.828280 -1.958950 0.297530
H -2.081250 -2.571730 0.410240
H -2.940490 -1.912660 -0.663680
O 1.371390 -1.920960 1.263780
H 0.973670 -1.071060 1.531890
H 1.897460 -1.680630 0.483640
O 2.656990 0.066830 -4.014650
H 2.171110 -0.708670 -4.403470
H 3.477180 0.142980 -4.511560
O 0.876140 2.270320 -3.876780
H 1.533150 1.567230 -4.043820
H 0.857680 2.322220 -2.906550
O -0.441050 -3.604960 0.281460
H -0.416800 -4.444140 0.750680
H 0.227770 -3.018800 0.725870

O 1.564130 1.283130 4.175150
H 2.024300 1.818770 4.828060
H 0.594190 1.470250 4.292410
O 1.089520 1.564070 -4.334860
H 1.349150 1.797040 -3.427240
H 1.399750 0.645990 -4.429810
O -1.461480 -1.327600 1.353220
H -1.752410 -1.515580 2.262910
H -0.494650 -1.478150 1.385430
O -1.461480 1.327600 -1.353220
H -0.494650 1.478150 -1.385430
H -1.752410 1.515580 -2.262910
O 1.564130 -1.283130 -4.175150
H 2.024300 -1.818770 -4.828060
H 0.594190 -1.470250 -4.292410
O -1.089520 1.564070 4.334860
H -1.349150 1.797040 3.427240
H -1.399750 0.645990 4.429810
O -1.358940 -1.480240 -1.495220
H -1.496100 -0.511150 -1.433610
H -1.671650 -1.803630 -0.636070
O 1.358940 1.480240 -1.495220
H 1.671650 1.803630 -0.636070
H 1.496100 0.511150 -1.433610

17-Pr454(4) O 4.394720 1.337760 -1.772130
H 4.336440 0.775390 -0.951060
H 5.263820 1.749170 -1.765430
O 0.236240 -1.839040 -0.402150
H -0.184900 -1.518740 -1.226260
H 1.098290 -2.186680 -0.694980
O -1.124990 2.901200 -3.663120
H -1.436690 3.559640 -4.290970
H -0.863910 3.401190 -2.842420
O 1.753060 2.214500 -1.489640
H 2.725700 2.203690 -1.546370
H 1.469190 1.721340 -2.288420
O 0.923890 0.878230 -3.805030
H 0.331970 1.602200 -4.073490
H 0.314130 0.149140 -3.584260
O -3.149080 -0.257360 1.331030
H -2.744660 -1.155080 1.181430
H -3.520800 -0.284290 2.217970
O 3.975260 -0.245260 0.301890
H 3.716900 -1.075580 -0.136370
H 3.148630 0.062070 0.716490
O 3.391070 -0.702640 -3.487950
H 3.896060 0.003130 -3.044380
H 2.622410 -0.236220 -3.852460
O -0.958580 -0.912340 -2.765050
H -1.565790 -0.183140 -2.497040
H -1.557910 -1.669510 -2.876280
O -4.621590 -0.622020 -1.150610
H -4.362130 -0.513370 -0.219020
H -4.157060 0.113450 -1.585810
O 2.831580 -2.290410 -1.385550
H 2.992100 -1.763500 -2.213110
H 3.201920 -3.162690 -1.551870
O -0.395510 3.986110 -1.341790
H -0.903250 3.557030 -0.635560
H 0.481310 3.560330 -1.288220
O -2.175540 -2.676760 0.744450
H -2.556500 -2.896470 -0.122960
H -1.230210 -2.557870 0.539110
O -1.428920 1.818000 0.442500
H -0.544600 1.468370 0.663730
H -2.044000 1.229980 0.918400
O -3.090190 -2.669140 -2.028700
H -3.620210 -3.348800 -2.455630
H -3.724590 -1.953260 -1.762370

18-Pr44244 O 1.174260 -2.565060 -2.595620
H 1.598910 -2.330950 -3.444050
H 1.926170 -2.798610 -2.009240
O 1.783880 -1.336360 2.597430
H 2.329160 -0.707690 2.095500
H 2.012640 -2.195450 2.185750
O 2.528060 1.005850 -3.683710
H 1.817570 0.882640 -3.025200
H 3.306100 1.180210 -3.125980
O 4.668500 0.871580 -1.717450
H 4.964760 0.010720 -2.111040
H 5.447790 1.433890 -1.678580
O -1.636490 -0.277190 -0.807030
H -1.543120 -0.459240 0.144180
H -1.761740 -1.155850 -1.197670
O -1.342470 -3.096960 -1.746730
H -1.885950 -3.584580 -2.372470
H -0.464260 -2.977720 -2.173360
O 3.403150 -2.770420 -0.951330
H 3.321680 -1.917280 -0.472520
H 3.270110 -3.424000 -0.244040
O -0.502110 -3.793710 0.829820
H -0.846690 -3.803510 -0.081350
H -0.682240 -2.873620 1.126230
O 1.202330 -2.618670 5.061710
H 1.572560 -2.010740 4.397840
H 0.245360 -2.450450 5.008790
O 0.991380 0.051480 -1.558230
H 0.052870 0.136350 -1.277030
H 1.020570 -0.853670 -1.923480
O 5.174400 -1.548700 -2.812670
H 4.538480 -1.604160 -3.546480
H 4.805070 -2.159340 -2.151420
O 2.825110 -1.482860 -4.544110
H 2.813300 -1.540940 -5.504030
H 2.702480 -0.517340 -4.318220
O -0.912340 -1.235100 1.769390
H 0.020530 -1.090730 2.028960
H -1.356310 -1.430490 2.615750
O -1.346340 -4.819430 3.312040
H -0.453670 -5.098340 3.580610
H -1.239710 -4.641010 2.359690
O 1.498110 -5.005300 3.845830
H 1.451360 -4.160440 4.368020
H 1.933290 -5.648810 4.412890

O -2.592060 1.143420 -2.008810
H -2.326820 1.813860 -2.664060
H -2.170890 1.421290 -1.166440
O 1.171310 0.591890 0.709130
H 0.834590 -0.265840 0.382180
H 1.383540 1.110360 -0.092370

O 2.218680 -3.840320 1.364800
H 1.291460 -3.905770 1.052380
H 2.231460 -4.418730 2.147840
O 3.013640 -0.277980 0.287740
H 3.707400 0.262520 -0.128830
H 2.220140 -0.073340 -0.254180
O -1.576830 -2.340420 4.264760
H -2.342040 -2.229870 4.836790
H -1.585830 -3.288850 3.961290

19-Globular O -0.088230 2.895360 1.877300
H -0.409210 2.074090 2.290180
H -0.095700 2.690680 0.921970
O -1.294570 -0.162240 -1.802320
H -0.849310 0.681260 -1.559010
H -2.041770 0.080200 -2.358410
O 2.227210 0.164590 2.795940
H 2.447690 1.108130 2.920440
H 1.277370 0.094950 3.012220
O 2.846680 0.656180 -3.325130
H 2.660290 1.539600 -2.969030
H 3.554440 0.333200 -2.742600
O 0.756060 -2.517240 0.182820
H 1.459780 -2.901860 0.741960
H 0.922980 -2.925390 -0.689610
O 0.203190 1.884840 -0.760200
H 0.839370 1.193380 -0.453400
H 0.778170 2.486130 -1.267900
O 4.365430 -1.571100 2.789450
H 4.939650 -0.956680 2.302710
H 3.598440 -1.006240 3.002430
O 1.906270 -0.003160 0.052670
H 1.482320 -0.886140 -0.010530
H 2.071120 0.104730 1.013980
O 4.098060 3.293230 0.338820
H 4.680140 2.540590 0.533780
H 3.515580 3.317020 1.119570
O 4.454030 -2.908360 -1.159050
H 4.163190 -3.192990 -0.277390
H 3.674760 -3.100930 -1.708680
O 3.110910 -3.432500 1.357150
H 3.203530 -4.273540 1.814550
H 3.608290 -2.767310 1.906960
O 2.442880 2.943550 2.618950
H 2.570630 3.569530 3.338010
H 1.483250 3.018380 2.349860
O 4.430210 -0.153710 -1.030460
H 4.564200 -1.125760 -1.116290
H 3.518610 -0.086030 -0.673060
O 5.466930 0.786600 1.245670
H 5.225640 0.413870 0.358190
H 6.423340 0.894280 1.238850
O -1.583910 -1.198080 0.934370
H -0.873510 -1.837550 0.738180
H -1.717570 -0.763970 0.074850
O -0.558920 0.263950 2.898750
H -0.971130 -0.263900 2.158250
H -1.114540 0.103980 3.667490
O 0.866100 -1.297420 -3.519360
H 1.533870 -0.577090 -3.514380
H 0.119140 -0.957520 -2.999380
O 1.838750 -3.377400 -2.248210
H 1.671020 -4.174360 -2.759680
H 1.495540 -2.617450 -2.801660
O 2.469880 3.162760 -1.847490
H 2.609460 3.984620 -2.327070
H 3.099900 3.194590 -1.083100

Table S4. Comparison of harmonic vs. anharmonic vibrational frequencies of water monomer and dimer; data used to derive an empirical relation.

water	anharmonic ω (cm ⁻¹)	harmonic ω (cm ⁻¹)
monomer	1595	1648
	3657	3832
	3756	3943
dimer	1600	1653
	1618	1669
	3548	3718
	3626	3797
	3698	3881
	3714	3899

Table S5. X3LYP/aug-cc-pVTZ(-f) normal mode frequencies corresponding to water cluster O-H stretching modes.

Geometry	1- Monomer	2- Dimer	3- Cyclic	4- Cyclic	5- Cyclic	6- Prism	6- Cage	6- Book	6- Bag	6- Cyclic	6- Cyclic'
Frequencies (cm ⁻¹)	3809.7	3693.1	3544.8	3345.1	3312.2	3137.0	3147.5	3225.5	3152.7	3298.2	3312.5
	3909.6	3804.3	3607.4	3444.6	3396.8	3412.6	3409.8	3317.8	3250.0	3375.8	3376.6
		3883.1	3618.0	3444.9	3406.5	3516.2	3455.8	3357.4	3321.9	3377.4	3396.9
		3900.0	3874.1	3484.2	3450.7	3535.5	3502.2	3480.7	3576.6	3434.5	3437.0
			3878.2	3866.8	3461.2	3670.5	3563.0	3555.6	3596.4	3435.8	3455.0
			3879.6	3867.4	3864.8	3680.3	3666.7	3567.8	3630.9	3453.3	3464.3
				3867.7	3866.0	3728.0	3695.0	3705.1	3643.3	3866.4	3866.2
				3868.6	3867.5	3743.2	3731.0	3865.0	3863.5	3866.7	3867.4
					3871.8	3769.6	3864.6	3865.2	3865.9	3867.2	3869.5
					3874.2	3869.4	3869.8	3868.3	3870.8	3867.8	3870.9
						3871.0	3870.8	3868.9	3871.9	3868.1	3877.7
						3871.5	3878.9	3870.2	3874.9	3868.8	3878.9
Geometry	7- Prism'	8- D2d	8- S4	9- D2dDD	10- Prism	10- Prism'	10- Butterfly				
Frequencies (cm ⁻¹)	3107.7	3150.3	3132.4	3145.9	3056.0	3066.4	3051.1				
	3276.7	3176.2	3161.7	3173.8	3079.3	3115.1	3225.9				
	3380.8	3178.6	3193.4	3178.3	3157.1	3153.0	3354.1				
	3497.8	3244.7	3194.7	3241.4	3160.8	3210.3	3463.9				
	3567.9	3601.6	3596.0	3294.0	3400.3	3413.2	3489.9				
	3587.8	3602.0	3596.7	3599.2	3452.1	3448.5	3519.2				
	3650.1	3616.3	3598.5	3600.6	3572.4	3575.6	3536.0				
	3666.0	3617.0	3602.1	3610.3	3577.4	3580.3	3567.8				
	3691.1	3617.9	3624.4	3613.9	3593.6	3597.3	3583.0				
	3783.8	3621.6	3648.7	3616.9	3603.0	3618.3	3583.8				
	3859.6	3664.6	3650.1	3626.0	3635.1	3622.5	3616.8				
	3865.2	3664.9	3662.0	3660.5	3636.5	3643.7	3651.7				
	3868.2	3863.7	3862.2	3664.6	3644.6	3659.2	3682.8				
	3870.2	3863.9	3862.9	3861.8	3689.7	3702.2	3802.2				
		3864.1	3863.3	3862.3	3706.4	3715.2	3809.2				
		3864.5	3863.8	3862.4	3860.2	3859.4	3852.5				

3864.2	3862.1	3861.2	3860.1
3871.9	3864.1	3861.3	3867.2
	3864.2	3861.9	3868.3
	3866.3	3863.5	3880.8

Table S6. Experimentally determined vibrational frequencies of water clusters and corresponding harmonic vibrational frequencies estimated through an empirical scaling relation.

# waters	1	2	3	4	5	6	7	8	9	10
Measured frequencies (cm ⁻¹)	3657	3548	3533	3416	3360		3720	3727	3719	3723
	3756	3626	3726	3714	3714		3650	3557	3568	3568
		3698					3560	3528	3541	3542
		3714					3420	3087	3140	3129
							3310	3065	3101	3100
							3080		3066	3063
							2950			
Harmonic frequencies (cm ⁻¹)	3834	3715	3699	3571	3509		3903	3911	3902	3907
	3943	3801	3910	3897	3897		3827	3725	3737	3737
		3879					3728	3693	3708	3709
		3897					3575	3211	3269	3257
							3455	3187	3226	3225
							3203		3188	3184
							3061			